SYOE 6: Transport in Organics Materials

Time: Tuesday 14:30–16:15 Location: H32

Invited Talk SYOE 6.1 Tue 14:30 H32

Theory of polymer devices: OFETs and OLEDs — •Reinder Coehoorn — Philips Research Laboratories, High Tech Campus 4, 5656 AE, Eindhoven, The Netherlands

The main challenge in the development of microscopic transport models and device models for polymer organic field effect transistors (OFETs) and organic light emitting diodes (OLEDs) is to properly include the effects of structural and energetic disorder of the materials used. In this talk, first an overview is given of the various methods for modelling the mobility in disordered organic materials on a microscopic scale, using numerical Monte Carlo, Master Equation (ME), and analytical percolation models. From ME modelling, it is shown that disorder leads to a carrier concentration dependence of the effective steady state, and has important consequences for the frequency dependence of the complex impedance. Furthermore, it leads to a filamentary, rather then uniform current density, as quasi-3D-visualized in the talk. This is expected to affect the device efficiency and (potentially) the lifetime. Subsequently, recent experimental evidence will be presented that proofs the important role of disorder in polymer LEDs and FETs, including recent results on dual gate and ambipolar light emitting OFETs, and on blue polymer OLEDs. In the final part of the talk, an overview will be given of the various challenging questions to be solved, including the question below which (sub)layer thickness the "mobility" concept is no longer meaningful.

The results presented in this talk have been obtained in collaboration with D.M. de Leeuw (Philips Research), S.L.M. van Mensfoort, B. Ramachandhran and P.A. Bobbert (Eindhoven University of Technology) and E.C.P.Smits (University of Groningen).

SYOE 6.2 Tue 15:15 H32

Trapped-Space-Charge-Limited Currents in Organics — •Gernot Paasch[1], Paul Blom[2], Magda Mandoc[2], and Bert de Boer[2] — [1]IFW Dresden, Germany — [2]University of Groningen, The Netherlands

The Mott-Gurney law for space charge limited current (SCLC) has been modified early [1] to account for the presence of exponentially distributed traps. This expression has been widely used to analyse transport in organic light emitting diodes. However, the theory fails to describe the rather weak temperature dependence observed for electron transport, for instance in PPV derivatives [2]. There we have shown that the trap-limited SCLC law is essentially modified if the density of transport states is of Gaussian type. Here, we discuss the origin of this modification and present a detailed analysis of the modified law. In addition, we derive further modifications for different combinations of densities of states of both the transport states and the trap distribution. As a result, rather different dependencies of the current on voltage, layer thickness and temperature are possible. Consequently, one has to exercise care in order to obtain reliable trap parameters from SCLC.

[1] P. Mark and W. Helfrich, J. Appl. Phys. 33, 205 (1962).

[2] M. M. Mandoc, B. de Boer, G. Paasch, P. W. M. Blom, submitted.

SYOE 6.3 Tue 15:30 H32

Macroscopic and Microscopic Simulations of the Charge Transport in Conjugated Polymers — •Carsten Deibel[1], Maria Hammer[1], Andreas Baumann[1], Ingo Riedel[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians- — [2]Div. Functional Materials for Energy Technology, ZAE Bayern e.V., Am Hubland, 97074 Würzburg, Germany

The charge carrier mobility is a key characteristic for describing charge transport in disordered organic semiconductors. Its multiple dependencies, e.g. on temperature and electric field, can be understood by considering hopping transport in a gaussian density of states. Microscopically, the hopping process can be looked at by Monte Carlo simulations, with the density of states distribution as input, and the mobility as output parameter. Macroscopically, the numerical solution of the Poisson equation can be utilised. Despite their different approaches, both models are able to give insight into charge transport in conjugated polymers. The application of the simulation results of these two models to experimentally observed transient photoconductivity and space charge limited current experiments of polymer devices will be discussed.

SYOE 6.4 Tue 15:45 H32

Charge mobility of discotic mesophases of hexabenzocoronene derivatives: a multiscale quantum/classical study of the effects of side chain substitution and temperature — •Denis Andrienko[1], Valentina Marcon[1], Kurt Kremer[1], James Kirkpatrick[2], and Jenny Nelson[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz — [2]Department of Physics, Imperial College London, Prince Consort Road, London SW7 2BW, United Kingdom

Discotic liquid crystals form columnar phases, where the molecules stack on top of each other and the columns arrange in a regular lattice. The self-organization into stacks results in the one-dimensional charge transport along the columns. Using atomistic molecular dynamics (MD) simulations we study the solid and liquid crystalline columnar discotic phases formed by the alkyl-substituted hexabenzocoronene mesogens. Correlations between the molecular structure, packing, and dynamical properties of these materials are established. Combining Kinetic Monte Carlo and MD trajectories a correlation between the material morphology and charge mobility is then obtained. We are able to reproduce the trends and magnitudes of mobilities as measured by pulse-radiolysis time-resolved microwave conductivity technique.

SYOE 6.5 Tue 16:00 H32

Trap-Controlled Hole Transport in a Small Molecule Organic Semiconductor — •Arne Fleissner, Hanna Schmid, Roland Schmechel, Christian Melzer, and Heinz von Seggern — TU Darmstadt, Institute of Materials Science, Electronic Materials Department, Petersenstr. 23, 64287 Darmstadt, Germany

The transport of charge carriers through organic semiconductors is strongly affected by trap states in the energy gap. In this work, a well defined concentration of hole traps is deliberately introduced into a small molecule hole transporter in order to control the mode of charge carrier transport and mobility. For that purpose, the host material N,N'-di(1-naphtyl)-N,N'-diphenylbenzidine (α-NPD) is molecularly doped by thermal co-evaporation with 4,4',4"-tris-[N-(1-naphtyl)-N-(phenylamino)]-triphenylamine (1-NaphDATA), which is known to create 0.4eV-deep neutral hole traps. Using a mechanical chopper to control the mass flow of the dopant, doping concentrations as low as 100ppm were achieved. The influence of the trap concentration on charge transport and mobility is studied on diode-like structures by an optical time-of-flight method. Non-dispersive hole transport is observed for undoped α-NPD. The introduction of 100ppm hole traps results in non-dispersive but trap-controlled transport and reduces the mobility by orders of magnitude. For increasing the trap concentration to over 1000ppm, the transition to dispersive transport is observed.